

On certain sum rules for the hydrogen atom

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Abstract. We show that some sum rules for the hydrogen atom derived recently are incorrect because the authors did not take into account the continuous part of the spectrum in the sum over intermediate states.

1. Introduction

Chair and Dalabeeh[1] and more recently Chair et al[2] derived sum rules for the hydrogen atom by means of the Rayleigh–Schrödinger perturbation theory. To this end, they compared the explicit sum over intermediate states with the exact result provided by the method of Dalgarno and Lewis[3].

The purpose of this paper is the analysis of those sum rules. In section 2 we outline the method of Dalgarno and Lewis and derive a general sum rule. In section 3 we discuss the validity of the sum rules derived by Chair and Dalabeeh[1] and Chair et al[2]. Finally, in section 4 we draw conclusions.

2. Perturbation theory

Suppose that we split the hamiltonian operator $H = H_0 + H'$ into the unperturbed H_0 and perturbation parts H' as is customary in Rayleigh–Schrödinger perturbation theory. We assume that we can solve the eigenvalue equation for H_0

$$H_0 |n\rangle = E_n^{(0)} |n\rangle, \quad n = 0, 1, \dots \quad (1)$$

where $E_0 < E_1 \leq E_2 \leq \dots$. The first and second order perturbation corrections to the ground–state energy (assumed to be nondegenerate) are

$$\begin{aligned} E_0^{(1)} &= \langle 0 | H' | 0 \rangle \\ E_0^{(2)} &= \sum_{n>0} \frac{|\langle n | H' | 0 \rangle|^2}{E_0^{(0)} - E_n^{(0)}} \end{aligned} \quad (2)$$

where

$$\sum_{n=0} |n\rangle \langle n| = \hat{1} \quad (3)$$

is the identity operator. If H_0 exhibits continuous spectrum then the sums above should include the corresponding integrals over such states[3].

The method of Dalgarno and Lewis[3] enables one to obtain the sum in equation (2) in closed form. If we can find an operator F such that

$$H' |0\rangle = [H_0, F] |0\rangle \quad (4)$$

then we obtain the sum rule

$$\sum_{n>0} \frac{|\langle n | H' | 0 \rangle|^2}{E_0^{(0)} - E_n^{(0)}} = \langle 0 | H' F | 0 \rangle - \langle 0 | H' | 0 \rangle \langle 0 | F | 0 \rangle \quad (5)$$

provided that the set of eigenfunctions satisfies (3).

3. The sum rules for hydrogen

In order to obtain their sum rules Chair and Dalabeeh[1] and Chair et al[2] proved that $\langle 0 | H' | 0 \rangle = 0$ and managed to calculate the matrix elements $\langle n | H' | 0 \rangle$ and $\langle 0 | H' F | 0 \rangle$ that appear in equation (5). However, since they omitted the continuous spectrum of hydrogen the bound states in their sums do not span the whole state space (that is to say: do not satisfy equation (3)) and, consequently, their sum rules cannot be exact.

We first analyse the sum rule derived by Chair et al[2]

$$S = 2^{10} \sum_{n=3}^{\infty} n^7 (n^2 - 4) \frac{(n-1)^{2n-6}}{(n+1)^{2n+6}} = \frac{15}{2} \quad (6)$$

If we take into account that

$$\frac{(n-1)^{2n-6}}{(n+1)^{2n+6}} < \frac{1}{(n+1)^{12}} \quad (7)$$

then we derive the inequality

$$\begin{aligned} S &< 2^{10} \sum_{n=3}^{\infty} \frac{n^7 (n^2 - 4)}{(n+1)^{12}} = -19456\zeta(11) - 57344\zeta(9) + 43008\zeta(7) \\ &\quad + 32768\zeta(5) + 1024\zeta(3) + \frac{707584\pi^{12}}{212837625} \\ &\quad + \frac{16384\pi^{10}}{31185} + \frac{1024\pi^8}{675} - \frac{8192\pi^6}{135} - \frac{512\pi^4}{5} + \frac{3}{4} \\ &\approx 6.889304238 \end{aligned} \quad (8)$$

where $\zeta(s) = \zeta(s, 1)$ and

$$\zeta(s, q) = \sum_{j=0}^{\infty} \frac{1}{(j+q)^s} \quad (9)$$

is the zeta function. We appreciate that $S < 6.889304238$ is considerably smaller than the result (6) given by Chair et al [2]. These authors compared their sum rule with one of those derived earlier by Bell[4]. However, Bell obtained the results of the sums and did not calculate the terms in the series explicitly. Chair et al[2] did it but only for the discrete states; for this reason their explicit sum rule is incorrect.

Chair and Dalabeeh[1] derived the following sum rule

$$S = \frac{2^8}{3} \sum_{n=2}^{\infty} n^5 \frac{(n-1)^{2n-4}}{(n+1)^{2n+4}} = 1 \quad (10)$$

In this case we slightly modify the strategy applied to the previous example. Note that

$$\begin{aligned} \frac{2^8}{3} \sum_{n=m+1}^{\infty} n^5 \frac{(n-1)^{2n-4}}{(n+1)^{2n+4}} &< \frac{2^8}{3} \sum_{n=m+1}^{\infty} \frac{n^5}{(n+1)^8} = \\ &= -\frac{256\zeta(8, m+2)}{3} + \frac{1280\zeta(7, m+2)}{3} - \frac{2560\zeta(6, m+2)}{3} \\ &\quad + \frac{2560\zeta(5, m+2)}{3} - \frac{1280\zeta(4, m+2)}{3} \\ &\quad + \frac{256\zeta(3, m+2)}{3} \end{aligned} \quad (11)$$

and that

$$S < S_m = \frac{2^8}{3} \sum_{n=2}^m n^5 \frac{(n-1)^{2n-4}}{(n+1)^{2n+4}} + \frac{2^8}{3} \sum_{n=m+1}^{\infty} \frac{n^5}{(n+1)^8} \quad (12)$$

where, obviously, $S_{m+1} < S_m$. Since $S_7 = 0.9461580468$ prove that S is smaller than unity.

4. Conclusions

We have proved that the sum rules derived by Chair and Dalabeeh[1] and Chair et al[2] are incorrect because the authors did not take into account the continuous spectrum of the hydrogen-atom Hamiltonian H_0 . Although those authors may have calculated the result of the sum exactly by means of the method of Dalgarno and Lewis[3] they omitted

the contribution of the continuous spectrum in the sum over intermediate states (5).

Therefore, their sums are always smaller than the exact results because

$$\sum_{n>0}^{discrete} \frac{|\langle n | H' | 0 \rangle|^2}{E_n^{(0)} - E_0^{(0)}} < \langle 0 | H' | 0 \rangle \langle 0 | F | 0 \rangle - \langle 0 | H' F | 0 \rangle$$

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- [4] Bell R J 1967 *Proc. Phys. Soc.* **92** 842.